

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010821\
 Data File : BG047901.D
 Acq On : 9 Jan 2021 00:45
 Operator : CG/JU
 Sample : M1044-18
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-11

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047901.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.509	24	29	39	rVB	60169	79736	2.30%	0.563%
2	4.707	228	233	241	rVB	100183	139435	4.03%	0.984%
3	5.177	307	313	316	rBV	66013	97514	2.82%	0.688%
4	5.213	316	319	325	rVB	25794	36635	1.06%	0.258%
5	5.747	403	410	424	rVB	862536	1487709	42.95%	10.495%
6	7.398	683	691	705	rBV	711008	1631070	47.09%	11.507%
7	8.162	814	821	830	rBV	170012	292959	8.46%	2.067%
8	9.331	1012	1020	1029	rBV	600592	1059241	30.58%	7.473%
9	10.988	1294	1302	1314	rVB	200496	358297	10.34%	2.528%
10	13.415	1708	1715	1722	rBV	1034148	1602619	46.26%	11.306%
11	14.231	1849	1854	1861	rVB2	30472	42747	1.23%	0.302%
12	14.790	1943	1949	1957	rBV2	220912	357481	10.32%	2.522%
13	16.282	2196	2203	2214	rBV	1085294	1635266	47.21%	11.536%
14	17.533	2408	2416	2422	rBV	341872	518044	14.96%	3.655%
15	20.124	2851	2857	2866	rBV	2706893	3464003	100.00%	24.438%
16	21.423	3073	3078	3091	rBV9	34661	87670	2.53%	0.618%
17	21.805	3137	3143	3152	rBV2	382359	646440	18.66%	4.560%
18	25.136	3699	3710	3721	rVB2	227290	637988	18.42%	4.501%

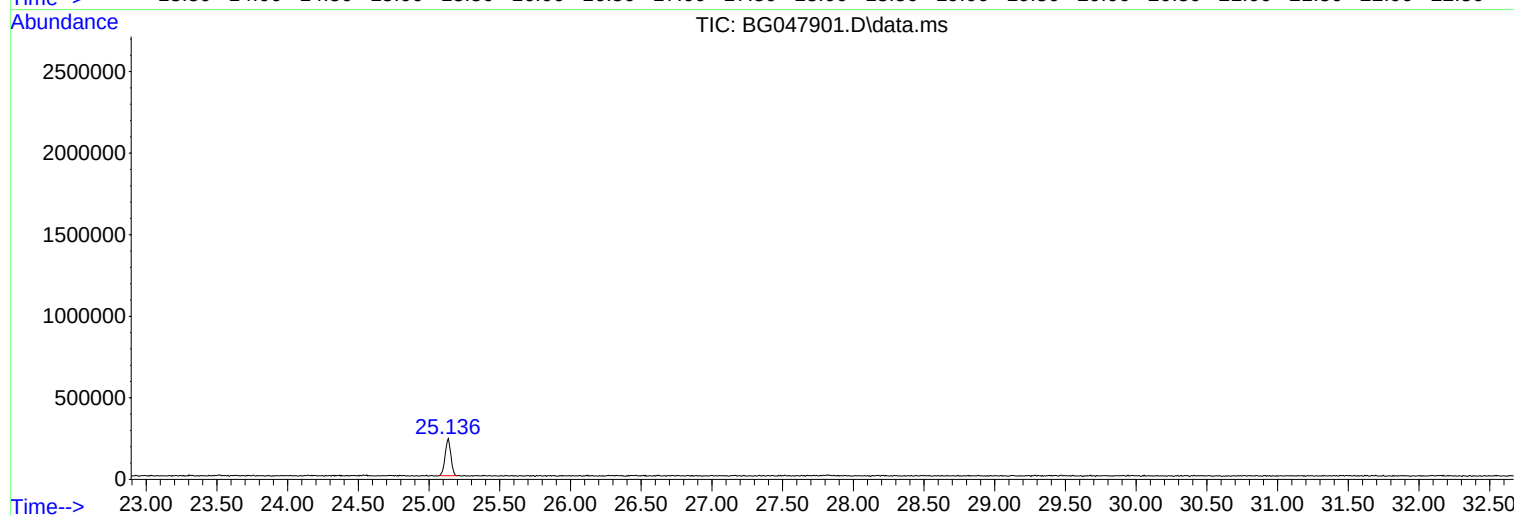
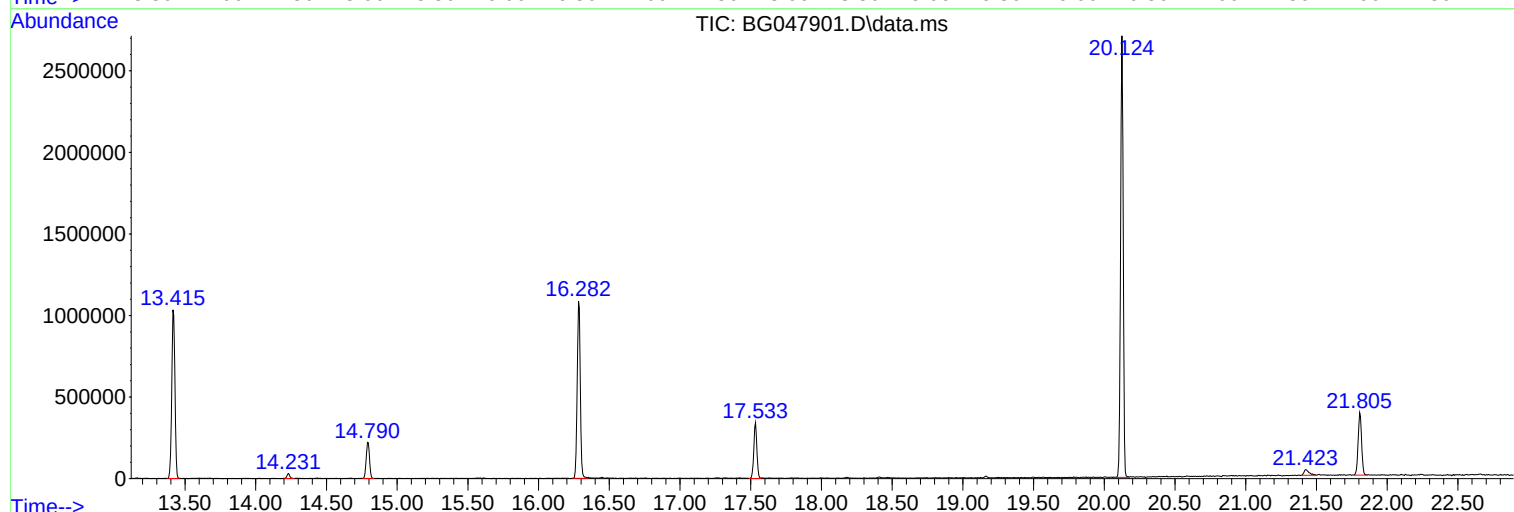
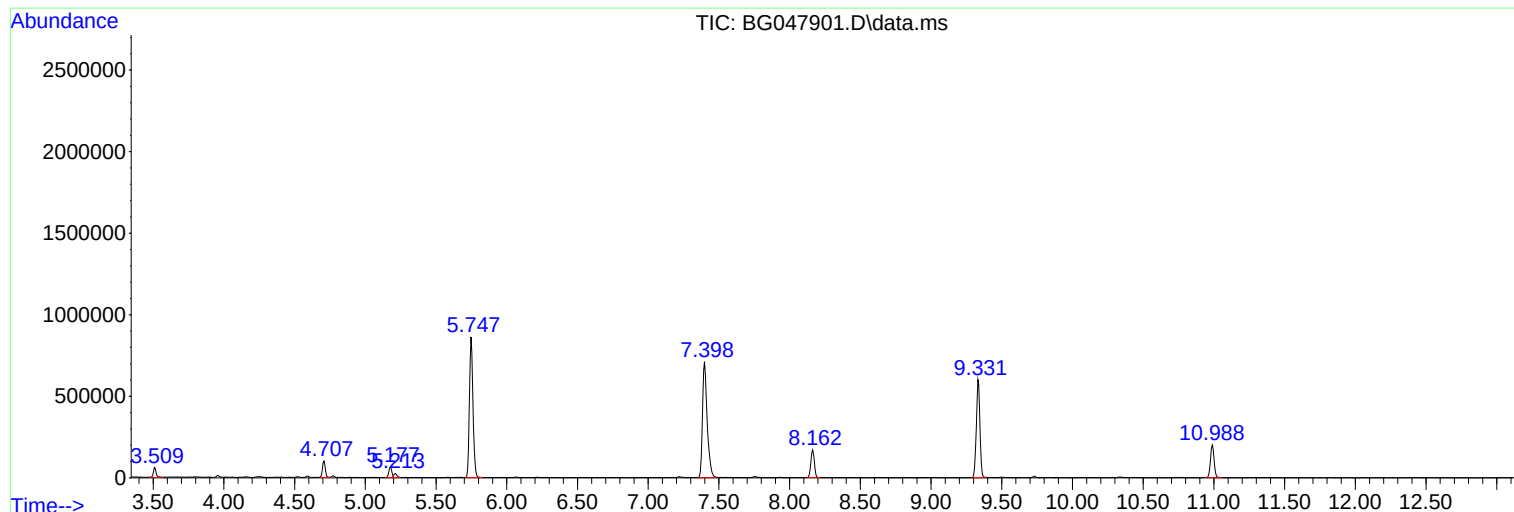
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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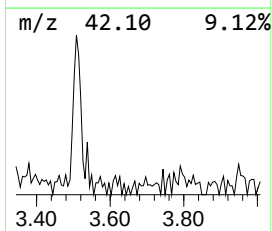
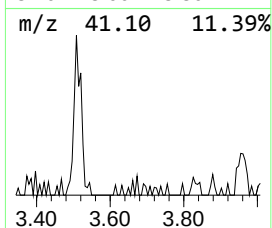
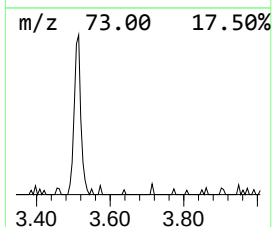
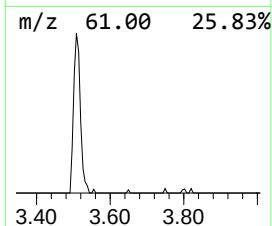
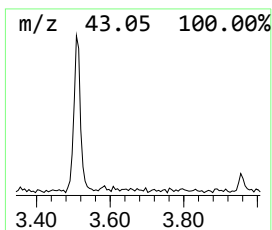
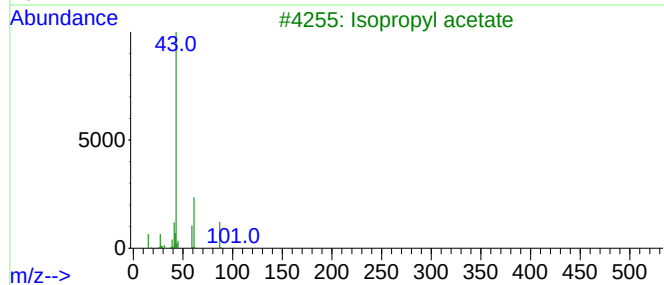
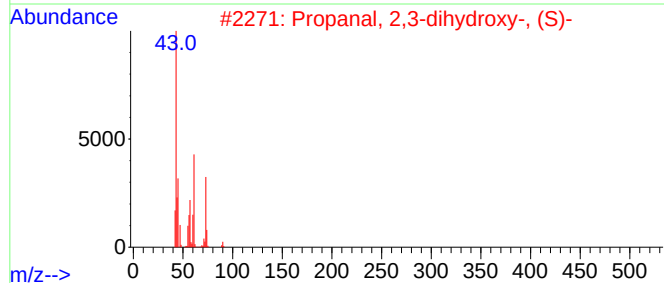
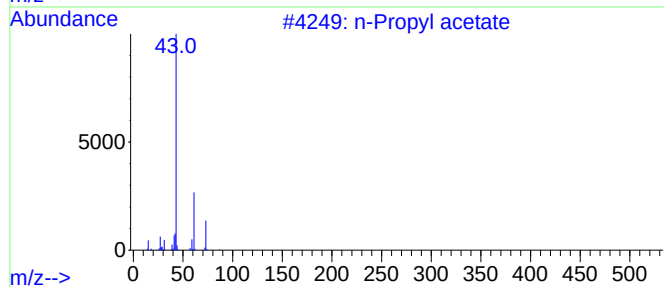
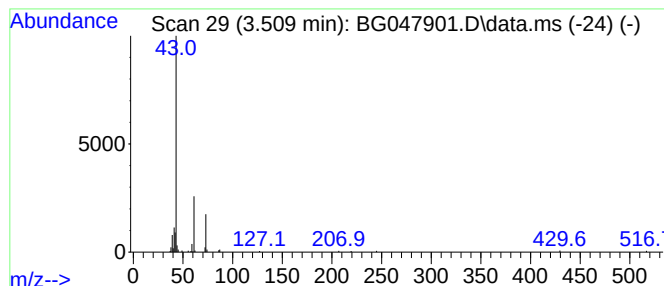
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.509	5.44 ng	79736	1,4-Dichlorobenzene-d4	8.162

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	64
2			Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	33
3			Isopropyl acetate	102	C5H10O2	000108-21-4	33
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			Di-n-propyl ether	102	C6H14O	000111-43-3	9



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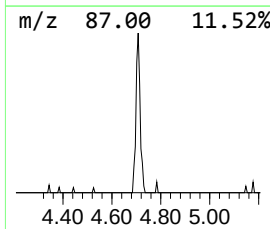
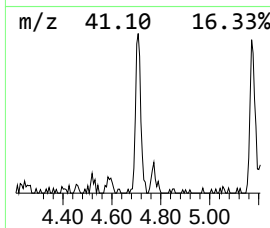
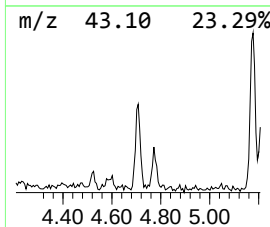
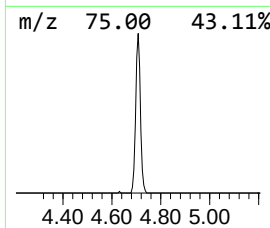
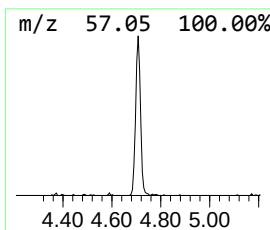
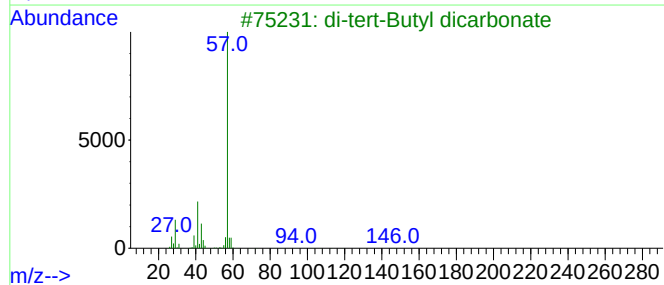
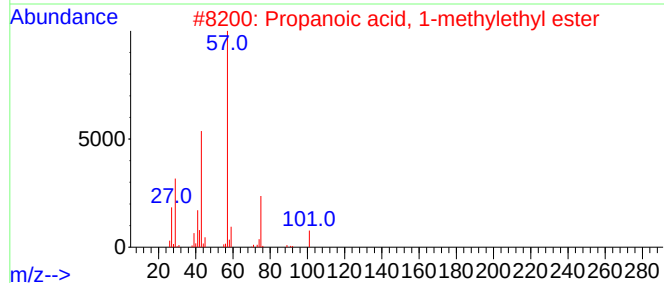
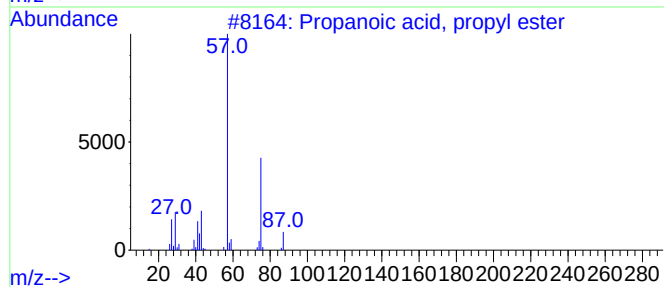
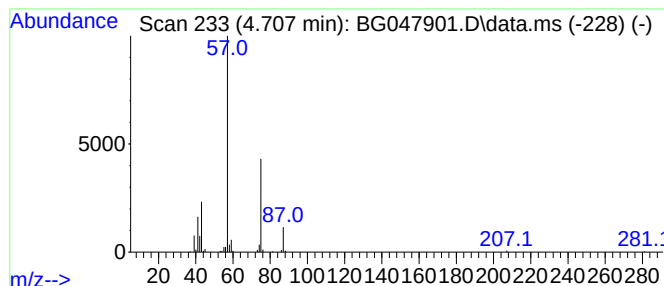
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.707	9.52 ng	139435	1,4-Dichlorobenzene-d4	8.162

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	25
3			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	14
4			1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	9
5			1-Butoxypropan-2-yl 2,2,2-triflu...	228	C9H15F3O3	1000367-08-1	9



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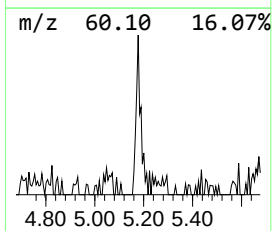
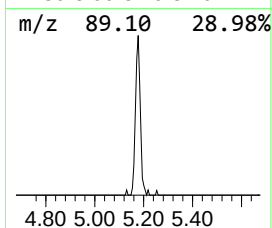
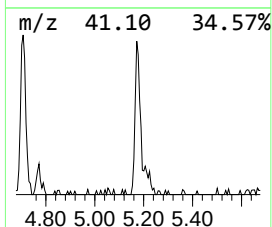
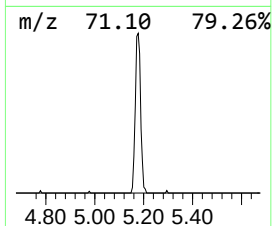
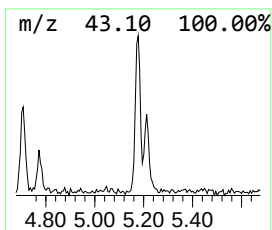
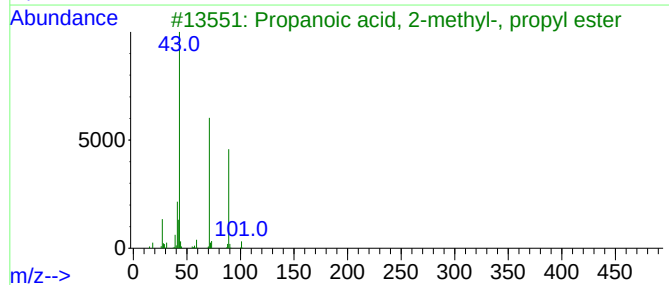
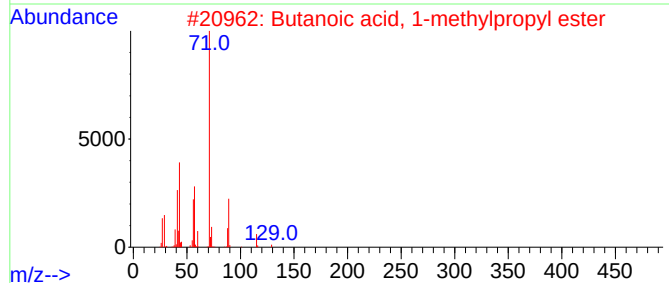
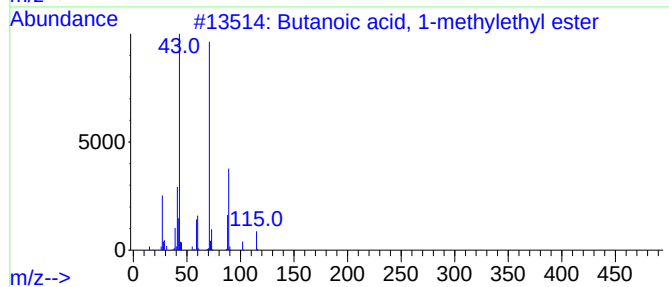
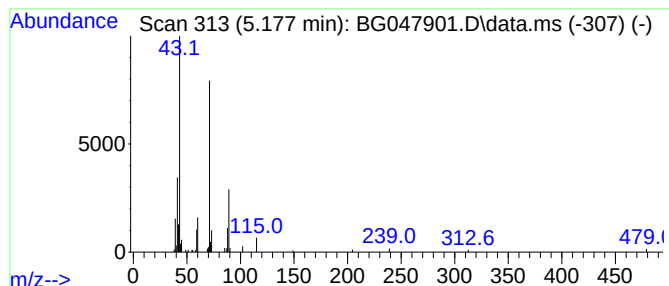
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Peak Number 3 Butanoic acid, 1-methylethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.177	6.66 ng	97514	1,4-Dichlorobenzene-d4	8.162

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	59



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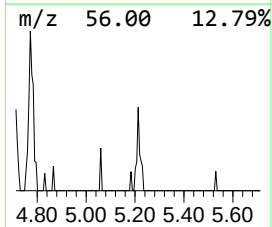
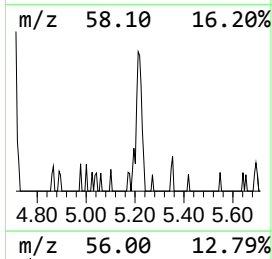
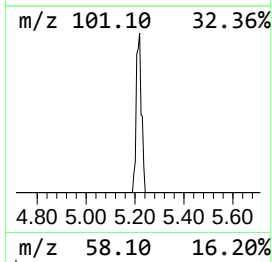
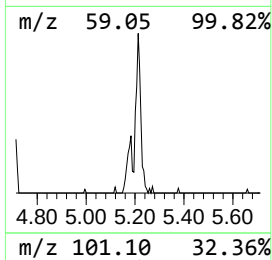
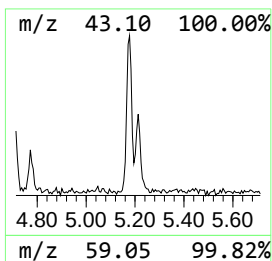
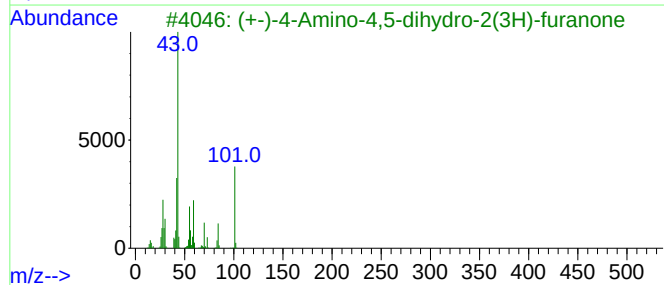
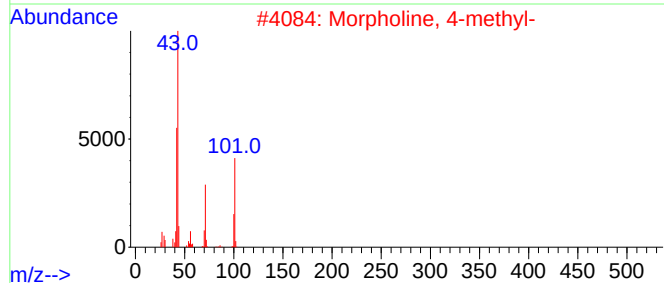
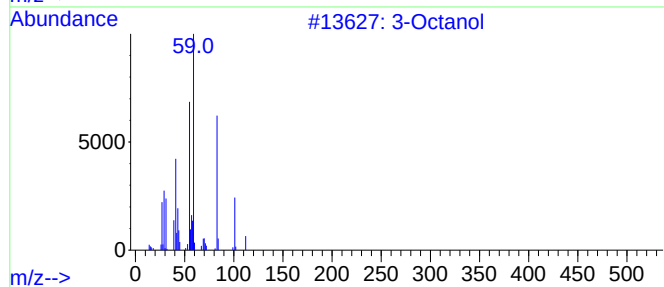
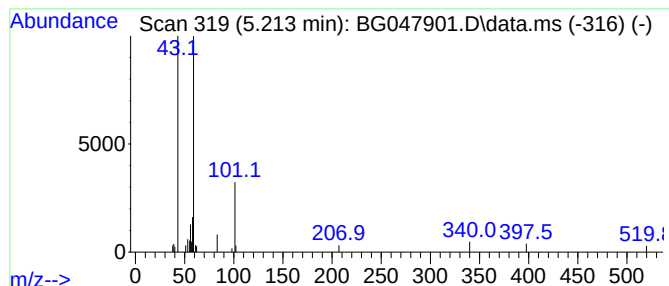
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Peak Number 4 unknown5.213 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.213	2.50 ng	36635	1,4-Dichlorobenzene-d4	8.162

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octanol	130	C8H18O	000589-98-0	38
2			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4			1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	9
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9



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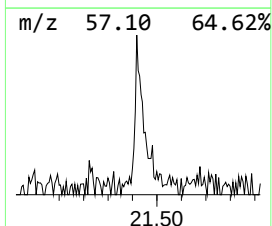
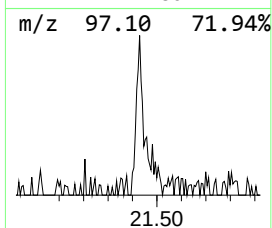
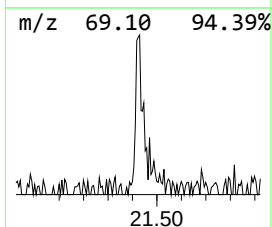
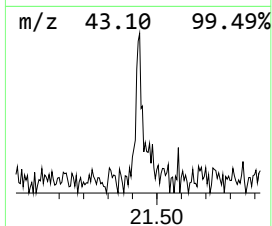
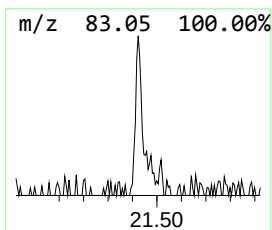
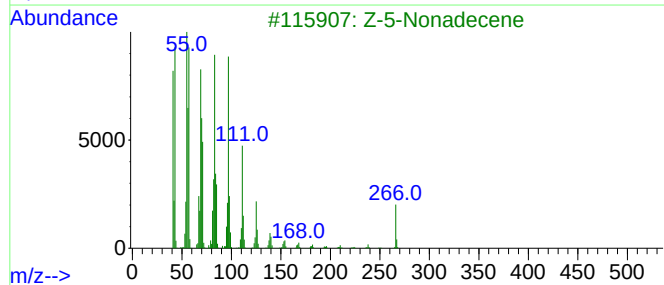
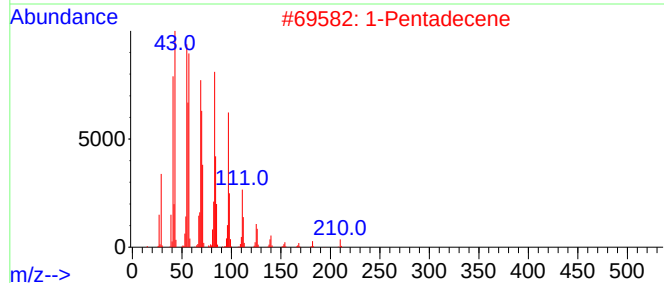
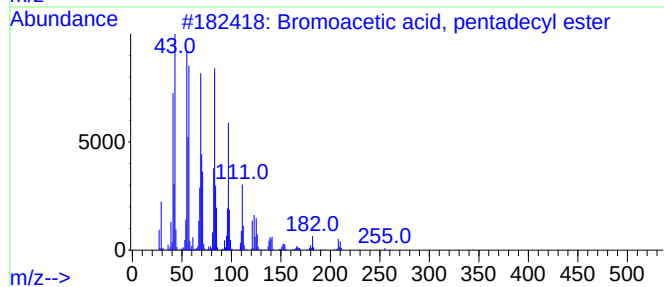
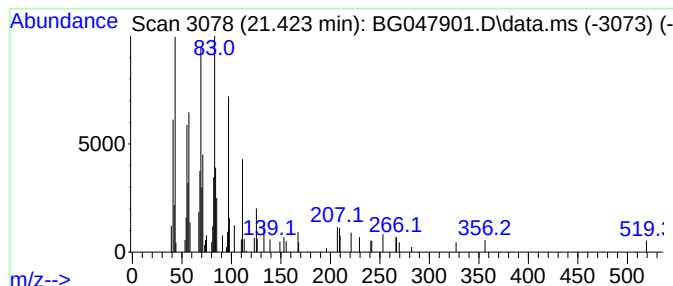
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Peak Number 5 Bromoacetic acid, pentadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.423	2.71 ng	87670	Chrysene-d12	21.805

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	90
2			1-Pentadecene	210	C15H30	013360-61-7	72
3			Z-5-Nonadecene	266	C19H38	1000131-11-8	68
4			1-Cyclopentyleicosane	350	C25H50	1000357-25-6	52
5			Cyclohexane, (1,3-dimethylbutyl)-	168	C12H24	061142-19-6	52



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	3.509	5.4	ng	79736	1	8.162	292959	20.0
Propanoic acid,...	4.707	9.5	ng	139435	1	8.162	292959	20.0
Butanoic acid, ...	5.177	6.7	ng	97514	1	8.162	292959	20.0
unknown5.213	5.213	2.5	ng	36635	1	8.162	292959	20.0
Bromoacetic aci...	21.423	2.7	ng	87670	5	21.805	646440	20.0